Superiority of semiclassical over quantum mechanical calculations for a three-dimensional system

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Abstract

In systems with few degrees of freedom modern quantum calculations are, in general, numerically more efficient than semiclassical methods. However, this situation can be reversed with increasing dimension of the problem. For a three-dimensional system, viz. the hyperbolic four-sphere scattering system, we demonstrate the superiority of semiclassical versus quantum calculations. Semiclassical resonances can easily be obtained even in energy regions which are unattainable with the currently available quantum techniques.

1 Introduction

The numerical calculation of quantum spectra is a nontrivial task especially for nonintegrable systems with many degrees of freedom. Rigorous computational methods have been developed for directly solving Schrödinger's equation, e.g., by time-dependent wave packet expansions or numerical diagonalization of the Hamiltonian in a complete basis set. Exact quantum mechanical calculations usually require storage of multidimensional wave functions and a computational effort that grows exponentially with the number of coupled degrees of

freedom. These methods are therefore feasible for systems with relatively few degrees of freedom. As an alternative to exact quantum calculations, approximate, e.g. semiclassical, methods can be applied. For systems with a chaotic classical dynamics Gutzwiller's trace formula expresses the quantum density of states in terms of the periodic orbits of the underlying classical system [1], i.e.,

$$\varrho(E) = \varrho_0(E) - \frac{1}{\pi} \operatorname{Im} \sum_{\text{po}} A_{\text{po}} e^{iS_{\text{po}}/\hbar} \, , \tag{1}$$

where $\varrho_0(E)$ is the mean density of states given by the phase space volume, and A_{po} and S_{po} are the amplitudes (including a phase given by the Maslov index) and classical actions of the classical periodic orbits (po), respectively. Eq. (1) can be applied to systems with an arbitrary number of degrees of freedom. However, the number of periodic orbits and the numerical effort needed to find them usually increases very rapidly with increasing dimension of the phase space. As a matter of fact, Gutzwiller's periodic orbit theory has been applied predominantly to systems with two degrees of freedom, e.g., the anisotropic Kepler problem [1,2], the hydrogen atom in a magnetic field [3], and two-dimensional billiards [4,5,6]. For these systems direct quantum mechanical computations are usually more powerful and efficient than the semiclassical calculation of spectra by means of periodic orbit theory. Practical applications of periodic orbit theory to three-dimensional systems are very rare. For the three-dimensional Sinai billiard extensive quantum computations have been performed and the quantum spectra have been analyzed in terms of classical periodic orbits [7,8]. However, no semiclassical eigenstates have been calculated from the set of periodic orbits. Semiclassical resonances have been obtained for the three-dimensional two- and three-sphere scattering systems [9] but for these systems all periodic orbits lie in a one- or two-dimensional subspace.

In this Letter we will, for the first time, calculate semiclassical resonances for a billiard system with genuinely three-dimensional periodic orbits, viz. the scattering of a particle on four equal spheres centered at the corners of a regular tetrahedron. Recently, experiments on chaotic light-scattering from the four-sphere system have attracted much attention [10,11]. An exact quantum mechanical recipe for the computation of resonances has been introduced in Ref. [9]. We will demonstrate that for this system semiclassical methods are superior to direct quantum mechanical computations, i.e., semiclassical resonances can easily be obtained even in energy regions which are unattainable with the presently known quantum techniques.

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2 The four-sphere scattering system

The four-sphere system can be regarded as the natural genuinely three-dimensional generalization of the two-dimensional three-disk system, which has served as the prototype model for classical, semiclassical, and quantum investigations of a chaotic repellor [12], as well as the development of cycle-expansion methods [4,5]. The periodic orbits of the symmetry reduced three-disk system can be described by a binary symbolic code, and allow us to compute the semiclassical resonances when Gutzwiller's trace formula (1) is combined, e.g., with the cycle-expansion [4,5] or harmonic inversion [13,14] technique. The semiclassical resonances are approximations to the exact quantum mechanical ones, which are obtained, e.g., in the A_1 subspace, as zeros of the determinant of the matrix [12,15]

$$\mathbf{M}(k)_{mm'} = \delta_{mm'} + d_m d_{m'} \frac{J_m(ka)}{H_{m'}^{(1)}(ka)} \left\{ \cos\left(\frac{\pi}{6}(5m - m')\right) H_{m-m'}^{(1)}(kR) \right.$$
$$\left. + (-1)^{m'} \cos\left(\frac{\pi}{6}(5m + m')\right) H_{m+m'}^{(1)}(kR) \right\} \tag{2}$$

with $0 \leq m, m' < \infty$ and

$$d_m = \begin{cases} \sqrt{2} \text{ for } m > 0 \\ 1 \text{ for } m = 0 \end{cases}.$$

In Eq. (2) a and R are the radius and center-to-center separation of the disks, k is the (complex) wave number, and $J_m(x)$ and $H_m^{(1)}(x)$ are Bessel and Hankel functions. The size of the matrix $\mathbf{M}(k)_{mm'}$ can be truncated by an upper angular momentum $m_{\max} \gtrsim 1.5ka$ [15]. For the frequently chosen disk separation $R = 6a$ both the semiclassical and quantum mechanical methods allow for the efficient computation of resonances in the region $0 \leq \mathrm{Re}\ ka \leq 250$.

In the three-dimensional four-sphere scattering system the computation of both the semiclassical and quantum mechanical resonances becomes more expensive. However, as will be shown below, the numerical effort required for the quantum calculations increases much more rapidly than that for the semiclassical. For identical spheres with radius a and equal separation R the discrete symmetry of the tetrahedral group, T_d, reduces the spectroscopy to five irreducible subspaces: A_1, A_2, T_1, T_2, and E [16]. We will perform all calculations for the A_1 subspace in what follows.

Exact quantum resonances of the four-sphere system can be obtained as roots of the equation

$$\det \mathbf{M}(k)_{lm,l'm'} = 0 \ , \tag{3}$$

with $0 \le l, l' \le l_{\max}$ and $m, m' = 0, 3, 6, 9, \ldots, l_{\max}$. The truncation value $l_{\max}$ for the angular momentum can be estimated by $l_{\max} \gtrsim 1.5ka$. The calculation of the matrix elements $\mathbf{M}(k)_{lm,l'm'}$ is rather complicated, as compared to the simple result in Eq. (2). Explicit expressions are given in Ref. [9]. (Note that $g_{m=0}$ should read $g_0 = 1/\sqrt{2}$ instead of $\sqrt{2}$ in Eq. (38) of [9].) However, the serious problem of solving Eq. (3) is the scaling of the dimension of the matrix $\mathbf{M}(k)_{lm,l'm'}$, which is an $N \times N$ matrix with $N = (l_{\max} + 2)(l_{\max} + 3)/6$, i.e., N scales as $N \sim k^2$ for the four-sphere system, as compared to $N \sim k$ for the three-disk system, Eq. (2). For example, in the region $ka \approx 200$ the required matrix dimension is $N \gtrsim 300$ for the three-disk compared to $N \gtrsim 15000$ for the four-sphere system. With currently available computer technology it is, therefore, impossible to significantly extend the quantum calculations for the four-sphere system to the region $ka \gg 50$ using the method of Ref. [9].

The computation of resonances in the region, e.g., $ka \le 250$ is, however, not a problem when periodic orbit theory is used. Eq. (1) is valid for the four-sphere system with the periodic orbit sum now including all three-dimensional periodic orbits which are scattered between the four spheres. In full coordinate space each periodic orbit can be described by a symbolic code given by the sequence of spheres where the orbit is scattered. Due to the T_d symmetry of the problem each orbit can be symmetry reduced to the fundamental domain. The symmetry reduced orbits can be described by a ternary alphabet of symbols '0', '1', and '2', which are the three fundamental orbits, i.e., the symmetry reductions of the shortest orbits scattered between two, three, and four spheres, respectively. We shall use the symbol '0' for returning back to the previous sphere after one reflection, symbol '1' for the reflection to the other third sphere out of the incident direction but in the same reflection plane of the orbit, and symbol '2' for the reflection to the other fourth sphere out of the reflection plane of the orbit. The reflection plane is defined as the plane which contains the centers of the first three different spheres backward in the history of the itinerary code of the orbit. Note that orbit codes which contain only the symbols '0' and '1' lie in a two-dimensional plane, i.e., they correspond to the set of orbits with a binary symbolic code, which has been well-established for the three-disk system [4,5]. Orbits including the '2'-symbol are genuinely three-dimensional orbits. The periodic orbits can be invariant under certain rotations and reflections. Each orbit can be assigned one of the symmetry elements $\{e, \sigma_d, C_2, C_3, S_4\}$ of the group T_d. Symmetry reduced orbits in the fundamental domain are two-, three-, or four-times shorter than the orbit in the full coordinate space when they belong to the symmetry class $\{\sigma_d, C_2\}$,

C_3, or S_4, respectively. The length of orbits belonging to symmetry class e is unchanged under symmetry reduction.

For the numerical calculation of the periodic orbits we vary, for a given symbolic code, the reflection points on the spheres until the physical length of the orbit becomes a minimum. Note that for an orbit with symbol length n the number of variational parameters is $2n$ for the four-sphere system, as compared to n parameters for the three-disk system. Despite this, the periodic orbit search remains numerically very efficient. In chaotic systems the number of periodic orbits increases exponentially. For the three-disk system the number of orbits with cycle length n is given approximately by $N \sim 2^n/n$ whereas it scales as $N \sim 3^n/n$ for the four-sphere system. Nevertheless, orbits up to a sufficiently high cycle length can be obtained. For a sphere separation of $R = 6a$ we have calculated the complete set of primitive periodic orbits with cycle length $n \leq 14$, numbering 533830 orbits in total. More details about the symbolic code, the symmetry properties, and the numerical computation of the periodic orbits will be given elsewhere.

The calculation of the periodic orbit amplitudes A_{po} in (1) requires the knowledge of the monodromy matrices and the Maslov indices of the orbits. The Maslov index increases by 2 at each reflection on a hard sphere, i.e., $\mu_{\mathrm{po}} = 2n$ for an orbit with cycle length n. The calculation of the monodromy matrix $\mathbf{M}_{\mathrm{po}}$ for the periodic orbits of three-dimensional billiards has been investigated in Refs. [8,17]. $\mathbf{M}_{\mathrm{po}}$ is a symplectic (4×4) matrix with eigenvalues λ_1, $1/\lambda_1$, λ_2, and $1/\lambda_2$. For the hyperbolic four-sphere system λ_1 and λ_2 are either both real or the orbits are loxodromic, i.e., the eigenvalues of $\mathbf{M}_{\mathrm{po}}$ are a quadruple $\{\lambda, 1/\lambda, \lambda^*, 1/\lambda^*\}$ with λ being a complex number. The periodic orbit sum for the four-sphere system then reads

$$g(k) = \sum_p \sum_{r=1}^{\infty} \frac{(-1)^{rn_p} L_p \mathrm{e}^{\mathrm{i}krL_p}}{\sqrt{|(2 - \lambda_{p,1}^r - \lambda_{p,1}^{-r})(2 - \lambda_{p,2}^r - \lambda_{p,2}^{-r})|}} \, , \tag{4}$$

where n_p is the cycle length, L_p the physical length, $\lambda_{p,i}$ are the eigenvalues of the monodromy matrix, and r is the repetition number of the primitive periodic orbit p. The parameters for the primitive periodic orbits with cycle length $n_p \leq 3$ are given in Table 1.

The semiclassical resonances of the four-sphere system are given by the poles of the function $g(k)$. However, it is well known that the periodic orbit sum (4) does not converge in those regions where the physical poles are located. For the three-disk system the cycle-expansion method [4,5,15] and harmonic inversion techniques [13,14] have proven to be powerful approaches for overcoming the convergence problems of the periodic orbit sum, and both methods can also be successfully applied to the four-sphere system.

Table 1

Parameters of the symmetry reduced primitive periodic orbits p with cycle length $n_p \leq 3$ of the four-sphere system with radius $a = 1$ and center-to-center separation $R = 6$.

p	sym	L	Re λ_1	Im λ_1	Re λ_2	Im λ_2
0	σ_d	4.000000	9.89898	0.00000	9.89898	0.00000
1	C_3	4.267949	-11.7715	0.00000	9.28460	0.00000
2	S_4	4.296322	-4.52562	9.49950	-4.52562	-9.49950
01	σ_d	8.316529	-124.095	0.00000	88.4166	0.00000
02	C_3	8.320300	-37.1479	98.0419	-37.1479	-98.0419
12	S_4	8.567170	117.644	0.00000	-102.992	0.00000
001	C_3	12.321747	-1240.54	0.00000	868.915	0.00000
002	S_4	12.322138	-353.853	976.176	-353.853	-976.176
011	σ_d	12.580808	1449.55	0.00000	824.981	0.00000
012	C_2	12.617350	1192.83	0.00000	-1020.66	0.00000
021	C_3	12.584068	1201.43	0.00000	-996.800	0.00000
022	S_4	12.619948	-755.582	804.976	-755.582	-804.976
112	σ_d	12.835715	-496.339	1038.46	-496.339	-1038.46
122	C_3	12.863793	-1100.56	0.00000	1219.28	0.00000

The idea of the cycle-expansion method is to expand the Gutzwiller-Voros zeta function [1,18]

$$Z_{\mathrm{GV}}(k; z) = \exp\left\{ -\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(-z)^{rn_p} \mathrm{e}^{\mathrm{i}rkL_p}}{\sqrt{|\det(\mathbf{M}_p^r - \mathbf{1})|}} \right\} \tag{5}$$

as a truncated power series in z, where z is a book-keeping variable which must be set to $z = 1$. The semiclassical resonances are obtained as the zeros of the cycle-expanded zeta function (5).

The harmonic inversion method is briefly explained as follows. The Fourier transform of the function $g(k)$ in Eq. (4) yields the semiclassical signal

$$C^{\mathrm{sc}}(L) = \sum_p \sum_{r=1}^{\infty} \frac{(-1)^{rn_p} L_p \mathrm{e}^{\mathrm{i}rkL_p}}{\sqrt{|\det(\mathbf{M}_p^r - \mathbf{1})|}} \delta(L - rL_p) , \tag{6}$$

as a sum of δ functions. The central idea of semiclassical quantization by harmonic inversion is to adjust the semiclassical signal $C^{\mathrm{sc}}(L)$ with finite length

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$L \leq L_{\text{max}}$ to its quantum mechanical analogue

$$C^{\text{qm}}(L) = \sum_n d_n \mathrm{e}^{-\mathrm{i}k_n L} , \tag{7}$$

where the amplitudes d_n and the semiclassical eigenvalues k_n are free adjustable complex parameters. Numerical recipes for extracting the parameters $\{d_n, k_n\}$ by harmonic inversion of the δ function signal (6) are given in [19,20].

The quantum mechanical and semiclassical A_1-resonances of the four-sphere system with radius $a = 1$ and center-to-center separation $R = 6$ are presented in Fig. 1. The quantum resonances marked by the squares have been obtained by solving Eq. (3) with matrices $\mathbf{M}_{lm,l'm'}$ of dimension up to (1134×1134), which is sufficient only to obtain converged results in the region Re $k \lesssim 50$ (see Fig. 1a). By contrast, the semiclassical resonances can easily be obtained in a much larger region, e.g., Re $k \leq 250$ shown in Fig. 1b. The crosses mark the zeros of the cycle-expanded Gutzwiller-Voros zeta function (5). The cycle-expansion has been truncated at cycle length $n_{\text{max}} = 7$, which means that a total set of just 508 primitive periodic orbits are included in the calculation. The plus symbols mark the semiclassical resonances obtained by harmonic inversion of the periodic orbit signal (6) with signal length $L_{\text{max}} = 60$ constructed from the set of 533830 primitive periodic orbits with cycle length $n_p \leq 14$.

In the region Re $k \leq 50$ (Fig. 1a) the quantum and semiclassical resonances agree very well with a few exceptions. The first few quantum resonances in the uppermost resonance band are narrower, i.e., closer to the real axis than the corresponding semiclassical resonances. A similar discrepancy between quantum and semiclassical resonances has already been observed in the three-disk system [5,15]. Furthermore, in the region Re $k < 15$ and Im $k < -0.5$ several quantum resonances have been found (see the squares in Fig. 1a), which seem not to have any semiclassical analogue. These resonances are related to the diffraction of waves at the spheres, and its semiclassical description requires an extension of Gutzwiller's trace formula and the inclusion of diffractive periodic orbits [21,22]. The semiclassical resonances obtained by either harmonic inversion or the cycle-expansion method (the plus symbols and crosses in Fig. 1b, respectively) are generally in perfect agreement, except for the very broad resonances that lie deep in the complex plane, i.e., in the region Im $k \lesssim -0.8$.

For the four-sphere system with large separation $R = 6a$ between the spheres the cycle-expansion method is most efficient for the calculation of a large number of resonances. The reason is that the assumption of the cycle-expansion that the contributions of longer periodic orbits in the expansion of the Gutzwiller-Voros zeta function (5) are shadowed by pseudo-orbits composed of shorter periodic orbits is very well fulfilled. The harmonic inversion method
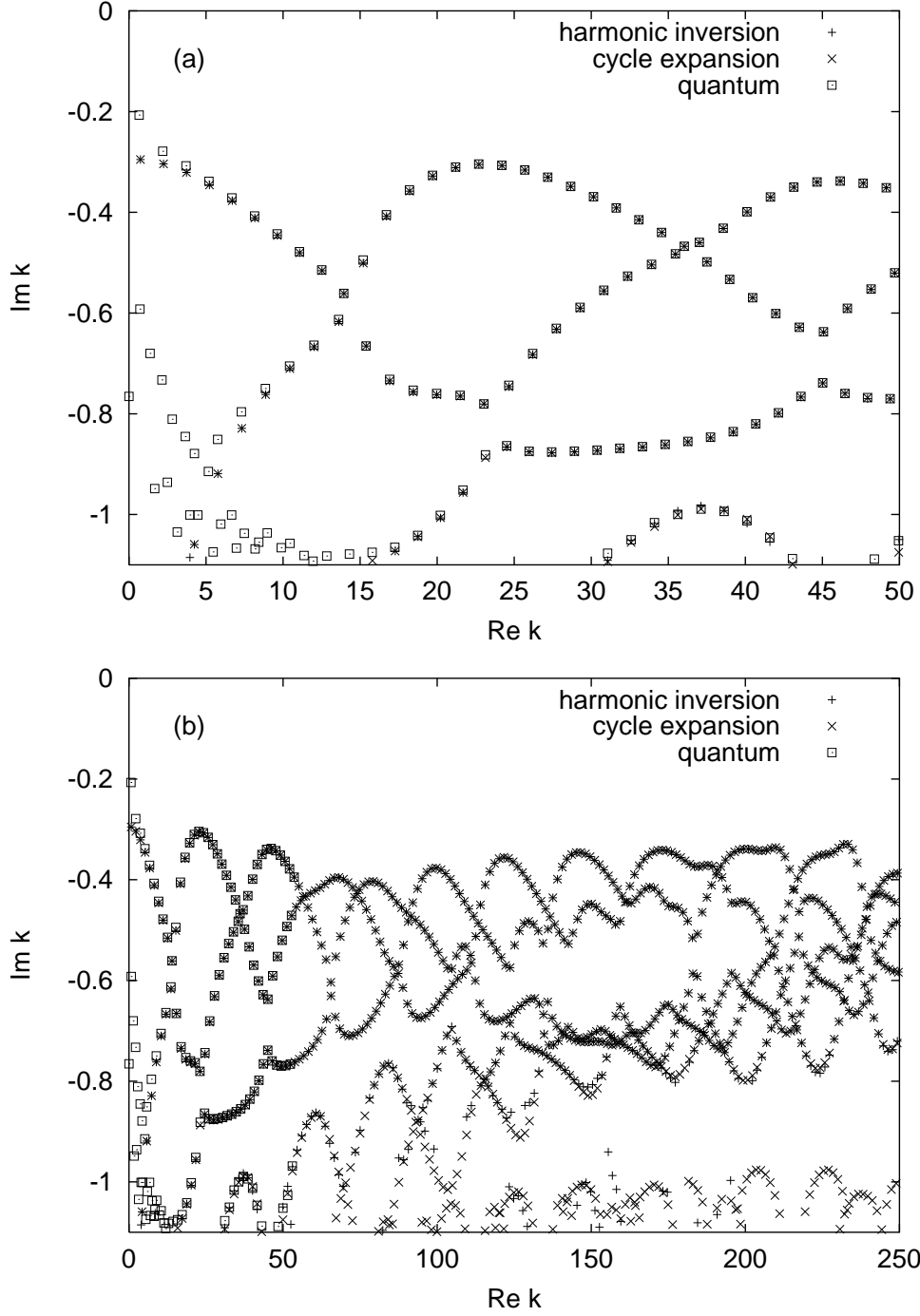
Fig. 1. A_1-resonances in the complex k-plane of the four-sphere system with radius $a = 1$ and center-to-center separation $R = 6$. Squares: Quantum computations. Crosses and plus symbols: Semiclassical resonances obtained by cycle-expansion and harmonic inversion methods, respectively.

also allows for the calculation of a large number of resonances, but requires a larger input set of periodic orbits. In contrast, the quantum computations for this three-dimensional system are very inefficient due to an unfavorable scaling of the dimension of the matrix $\mathbf{M}_{lm,l'm'}$ in Eq. (3). For this reason, the quantum computations presented here have been restricted to the region Re $k \leq 50$. Of course, a more efficient quantum method for the four-sphere system than that of Ref. [9] may in principle exist. However, to the best of our knowledge no such method has been proposed in the literature to date.

3   Summary and outlook

In summary, we have applied Gutzwiller's periodic orbit theory to a system with three degrees of freedom, viz. the four-sphere scattering problem. For the first time, semiclassical resonances have been obtained for a billiard system with genuinely three-dimensional periodic orbits. For this system we have discussed the scaling properties of both quantum and semiclassical calculations and have demonstrated the superiority of semiclassical methods over quantum computations, i.e., semiclassical resonances could easily be obtained in energy regions which are unattainable with the established quantum method. These results may encourage the investigation of other systems with three or more degrees of freedom with the goal to develop powerful semiclassical techniques, which are competitive with or even superior to quantum computations for a large variety of systems.

Interesting future work will also be the investigation of the four-sphere system when the spheres are moved towards each other. In particular, the case of touching spheres with $R = 2a$ is a real challenge, because the cycle-expansion does not converge any more. For touching spheres the symbolic dynamics is pruned in a similar way as in the three-disk problem [23]. However, contrary to the closed three-disk system [2,24], the four touching spheres do not form a bound system which means that the method of Ref. [2] combining the cycle-expansion method with a functional equation cannot be applied.

Acknowledgements

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